

### **AMENDMENTS TO THE CLAIMS:**

Please amend claims 37-40, 44, 46, 59, 60, 63, 133, 137, and 139-141, and add new claims 143-145 as indicated in the following listing of claims, which replaces all prior versions and listings of claims in the application:

#### **Listing of Claims:**

1. (Previously Presented) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to screening results from tests of interactions between each of a plurality of compounds in the first database and each of a plurality of molecular targets in the second database, the tests including information on the effect that a compound selected from the first database has on the interaction between a reference compound known to interact with a selected molecular target from the second database and said selected molecular target; and

a user interface allowing a user to view the selected compound and to selectively view information from the first database, the second database, and the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database.

2. (Original) The computer system of claim 1, wherein the interaction includes binding and the effect includes inhibitory effect.

3. (Previously Presented) The computer system of claim 1, wherein the chemical compounds include compounds with known biological activity.

4. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds that have been or are being tested in preclinical studies in animals.

5. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds known to have an effect on the environment.

6. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include pharmacological reference agents.

7. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include known pharmaceuticals in the market for clinical use for which there is a substantial amount of biological information available.

8. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include drug candidates approved by the Food and Drug Administration for testing in humans.

9. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds obtained from natural sources that exhibit biological activity.

10. (Original) The computer system of claim 1, wherein the molecular targets include receptors.

11. (Withdrawn) The computer system of claim 1, wherein the molecular targets include enzymes.

12. (Withdrawn) The computer system of claim 1, wherein the molecular targets include nucleic acids.

13. (Withdrawn) The computer system of claim 1, wherein the molecular targets include carbohydrates.

14. (Original) The computer system of claim 1, wherein the records of the first database corresponding to a plurality of chemical compounds are organized in categories related to the description and properties of the compounds.

15. (Original) The computer system of claim 14, wherein the categories include:  
compound name;

compound type;  
physical-chemical characteristics;  
chemical space coordinates or structural descriptors; and  
solubility.

16. (Original) The computer system of claim 1, wherein the first database includes a natural product database.

17. (Previously Presented) The computer system of claim 1, wherein the first database includes a database of chemical compounds that have failed in preclinical or human clinical tests.

18. (Original) The computer system of claim 1, wherein the first database includes a chemical registry database.

19. (Original) The computer system of claim 1, wherein the second database includes a three-dimensional structure database.

20. (Original) The computer system of claim 1, wherein the second database includes a sequence/mutation database.

21. (Original) The computer system of claim 1, wherein the second database includes a genomic database.

22. (Original) The computer system of claim 1, wherein the records in the third database corresponding to biological information related to the chemical compounds effects on the biological targets, are organized in categories that include:

compound name;

target name;

toxicity;

side effects; and

mechanism of drug action.

23. (Original) The computer system of claim 1 further comprising means for setting an interaction test threshold corresponding to said effect and means for selecting the compound when its use results in a test meeting the interaction test threshold.

24. (Withdrawn) A method for analyzing data relevant to drug discovery and development comprising:

selecting chemical compounds from a first database containing records corresponding to a plurality of chemical compounds;

selecting molecular targets from a second database containing records corresponding to a plurality of molecular targets;

producing information corresponding to the interactions between each of the selected chemical compounds and each of the selected molecular targets;

selecting a biological activity from a third database containing records corresponding to biological information related to effects of chemical compounds on biological targets; and

using the produced information to correlate patterns of interactions between chemical compounds and molecular targets associated with the selected biological activity.

25. (Withdrawn) The method of claim 24, wherein the step of producing information includes the steps of:

generating binding data of the binding between each of the selected chemical compounds and each of the selected molecular targets by monitoring the inhibitory effect that an unknown compound has on said binding;

setting a binding test threshold corresponding to the inhibitory effect; and

generating information on the combination of unknown compound, molecular target, and chemical compound that meets or fails to meet the binding test threshold.

26. (Withdrawn) The method of claim 25, wherein the binding data comprises positive and negative binding information.

27. (Previously Presented) The computer system of claim 1, wherein the interaction includes binding.

28. (Previously Presented) The computer system of claim 1, wherein the chemical compounds include compounds with known biological activity or that have failed in preclinical or human clinical tests.

29. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include compounds used in commerce as herbicides or pesticides.

30. (Withdrawn) The computer system of claim 1, wherein the chemical compounds include known pharmaceuticals approved for human clinical use by the Food and Drug Administration.

31. (Withdrawn) The computer system of claim 1, wherein the molecular targets include ion channels.

32. (Withdrawn) The computer system of claim 1, wherein the molecular targets include transporters or uptake sites.

33. (Previously Presented) A computer system comprising:  
a first database containing data corresponding to a plurality of chemical compounds;  
a second database containing data corresponding to a plurality of molecular targets;

a third database containing records corresponding to screening results from tests of interactions between each of a plurality of compounds in the first database and each of a plurality of molecular targets in the second database, the tests including information on the effect that a compound selected from the first database has on the interaction between a reference compound known to interact with a selected molecular target from the second database and said selected molecular target; and

a user interface allowing a user to view information from the first database, the second database, and the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database or as it relates to one or more interaction records in the third database.

34. (Previously Presented) The computer system of claim 33, wherein the chemical compounds include compounds with known biological activity.

35. (Previously Presented) A computer system comprising:

a first database containing data corresponding to a plurality of chemical compounds and data corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing data corresponding to a plurality of molecular targets;

a third database containing data corresponding to tests of interactions between each of a plurality of compounds in the first database and each of a plurality of molecular targets in the second database; and



a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.

36. (Previously Presented) The computer system of claim 35, wherein the chemical compounds include compounds with known biological activity.

37. (Currently Amended) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing records corresponding to a plurality of molecular targets; and

a third database containing records corresponding to screening results from tests of interactions between each of a plurality of compounds in the first database and each of a plurality of molecular targets in the second database, the tests including information on the effect that a compound selected from the first database has on the interaction between a reference compound known to interact with a selected molecular target from the second database and said selected molecular target; and

a user interface that allows a user to view information from at least one of the first database, the second database, and the third database.

38. (Currently Amended) The computer system of claim 37, ~~further comprising:~~  
wherein the a user interface allows ~~allowing~~ a user to view information from at least one of the first database, the second database, and the third database as it relates to a compound record in the first database.

39. (Currently Amended) The computer system of claim 37, ~~further comprising:~~  
wherein the a user interface allows ~~allowing~~ a user to view information from at least one of the first database, the second database, and the third database as it relates to a molecular target in the second database.

40. (Currently Amended) The computer system of claim 37, ~~further comprising:~~  
wherein the a user interface allows ~~allowing~~ a user to view information from at least one of the first database, the second database, and the third database as it relates to one or more interaction records in the third database.

41. (Previously Presented) The computer system of claim 37, wherein the interaction includes binding.

42. (Previously Presented) The computer system of claim 37, wherein the interaction includes binding and the effect includes inhibitory effect.

43. (Previously Presented) The computer system of claim 37, wherein the chemical compounds include compounds with known biological activity.

44. (Currently Amended) A memory for storing data for access by a process being executed by a processor, the memory comprising:

a data structure for maintaining (i) a first set of information associated with one or more chemical compounds, (ii) a second set of information associated with one or more molecular targets, and (iii) a third set of information reflecting interactions between each of a plurality of the chemical compounds and each of a plurality of the molecular targets, wherein the process may provide, based on one or more queries, new information reflecting a relationship between a chemical compound included in the first set, a molecular target included in the second set, and the information included in the third set, and wherein the information reflecting the relationship is relevant to a predictability of a potential use of a new compound.

45. (Previously Presented) In a system for correlating data associated with chemical compounds and molecular targets, a memory comprising:

a first array of records, each including information indicative of a chemical compound;

a second array of records, each including information indicative of a molecular target;

a third array of records, each corresponding to a binding capability between each of the chemical compounds and molecular targets; and

a fourth array of records, each corresponding to a biological activity related to the chemical compounds and the molecular targets,

wherein a process may access the first, second, and third arrays to produce information corresponding to a drug potential for a new compound based on relationships between characteristics associated with the new compound and a selected biological activity included in the fourth array of records or patterns of binding capabilities included in the third array.

46. (Currently Amended) A database for storing data for access by a process executed by a processor, the database comprising:

a compound data structure including data associated with a set of chemical compounds;

a target data structure including data associated with a set of molecular targets;  
and

a result data structure including data corresponding to results of screening tests between each of a plurality of chemical compounds from the set of chemical compounds and each of a plurality of molecular targets from the set of molecular targets,

wherein the process determines information reflecting a new relationship between the data included in the compound, target, and result data structures, and wherein the information reflecting the relationship is used to validate disease relevance or biological function of a new molecular target.

47. (Previously Presented) The database of claim 46, wherein the results include information on an effect a selected compound has on a known interaction of

another compound with a selected molecular target and an effect of the selected compound with the selected molecular target.

48. (Previously Presented) The database of claim 46, wherein the chemical compounds include at least one of:

- (i) compounds with known biological activity,
- (ii) compounds tested in animals,
- (iii) compounds known to have an effect on the environment,
- (iv) pharmacological reference agents,
- (v) known pharmaceuticals that have available preexisting biological information, and
- (vi) compounds approved by a government agency for testing in humans.

49. (Previously Presented) The database of claim 46, wherein the molecular targets include at least one of:

- (i) receptors,
- (ii) enzymes,
- (iii) nucleic acids,
- (iv) carbohydrates,
- (v) ion channels, and
- (vi) transporters or uptake sites.

50. (Previously Presented) The database of claim 46, wherein the process also provides a graphical interface including a description and properties of a selected chemical compound included in the compound data structure.

51. (Previously Presented) The database of claim 50, wherein the graphical interface includes a representation of at least one of the selected compound's name, type, structure, physical-chemical characteristics, chemical structural descriptors, and solubility.

52. (Previously Presented) The database of claim 46, including a biological data structure including information corresponding to biological information related to an effect of each chemical compound included in the compound data structure on each molecular target included in the target data structure.

53. (Previously Presented) The database of claim 52, wherein the biological information includes at least one of side effects, toxicity, and mechanism of drug action.

54. (Previously Presented) In a system for maintaining test screening results, a storage device for storing data for access by a process being executed by a processor comprising:

a data set including information corresponding to results of screening assay tests that measure an interaction between all possible combinations of chemical compounds

in a compound set and molecular targets in a molecular target set, thereby creating a full-rank data set of test results,

wherein the process provides selected result information based on a request associated with a selected chemical compound or molecular target.

55. (Previously Presented) The system of claim 54, wherein the results are represented in a form that reflects whether each chemical compound binds with a corresponding molecular target.

56. (Previously Presented) The system of claim 54, wherein the results are represented in a form that reflects a potency of a binding between each chemical compound and a corresponding molecular target.

57. (Canceled)

58. (Withdrawn) A system comprising:  
a memory including one or more data arrays of information associated with chemical compounds and molecular targets; and  
a processor for executing a process for providing a user interface including:  
a representation of a selected chemical compound,  
description information associated with the selected chemical compound, and  
biological information associated with the selected chemical compound.

59. (Currently Amended) A computer system comprising:

- a first database containing records corresponding to a plurality of chemical compounds; [[,]]
- a second database containing records corresponding to a plurality of molecular targets;
- a third database containing records corresponding to the results of tests to determine the interaction between each of a plurality of compounds in the first database and each of a plurality of targets in the second database; and
- a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.

60. (Currently Amended) The computer system of claim 59, wherein the third database includes records corresponding to the results of tests to determine the interaction between all of the compounds selected to comprise a compound set in the first database and ~~all or substantially~~ all of the molecular targets selected to comprise a molecular target set in the second database.

61. (Previously Presented) The computer system of claim 59, wherein the third database includes records corresponding to the results of tests to determine the interaction between a majority of the compounds selected to comprise a compound set



in the first database and a majority of the molecular targets selected to comprise a molecular target set in the second database.

62. (Previously Presented) The computer system of claim 59, further comprising:

a fourth database containing records corresponding to the effect of chemical compounds contained in the first database on biological systems.

63. (Currently Amended) The computer system of claim 62, wherein the third database includes records corresponding to the results of tests to determine the interaction between all of the compounds selected to comprise a compound set in the first database and ~~all or substantially~~ all of the molecular targets selected to comprise a molecular target set in the second database.

64. (Previously Presented) The computer system of claim 62, wherein the third database includes records corresponding to the results of tests to determine the interaction between a majority of the compounds selected to comprise a compound set in the first database and a majority of the molecular targets selected to comprise a molecular target set in the second database.

65. (Withdrawn) The computer system of claim 59, wherein the first database contains records corresponding to a plurality of known biologically active chemical compounds selected from among representatives of the following categories:

(a) pharmacological reference agents used in receptor, ion channel, transporter, or enzyme screening assays;

(b) drug candidates that have been approved by the Food and Drug Administration for testing in humans, including those that have been discontinued from further development; and

(c) pharmaceuticals that have been approved for human clinical use by the Food and Drug Administration, including those that have been subsequently withdrawn from the market.

66. (Withdrawn) The computer system of claim 65, wherein the known biologically active compounds included in the first database are further selected from among the following:

compounds that have been tested in preclinical studies in animals;

pesticides;

herbicides;

bioactive natural products;

agricultural chemicals; and

environmental chemicals.

67. (Previously Presented) The computer system of claim 59, wherein the second database contains records corresponding to a plurality of molecular targets selected from among representatives of the following categories:

(a) receptors;

- (b) ion channels;
- (c) transporters; and
- (d) enzymes.

68. (Previously Presented) The computer system of claim 65, wherein the second database contains records corresponding to a plurality of molecular targets selected from among representatives of the following categories:

- (a) receptors;
- (b) ion channels;
- (c) transporters; and
- (d) enzymes.

69. (Withdrawn) The computer system of claim 67, wherein the molecular targets in the second database are related to drug discovery and development.

70. (Previously Presented) The computer system of claim 59, wherein the third database contains records corresponding to complete sets of results from a screening process.

71. (Previously Presented) The computer system of claim 59, wherein the records in the third database corresponding to the results of tests to determine the interaction between compounds in the first database and targets in the second database includes positive interactions and negative or lack of interactions.

72. (Previously Presented) The computer system of claim 59, wherein the tests to determine the interaction between compounds in the first database and the targets in the second database are based on binding interactions.

73. (Previously Presented) The computer system of claim 59, wherein the tests to determine the interaction between compounds in the first database and the targets in the second database measure the inhibition of binding by a compound in the first database with respect to a target in the second database in the presence of another compound, such as a reference agent or enzyme substrate, known to interact with the target.

74. (Previously Presented) The computer system of claim 59, wherein the tests used to generate results comprising the third database are ligand binding assays.

75. (Previously Presented) The computer system of claim 59, wherein the tests used to generate results comprising the third database are enzyme inhibition assays.

76. (Previously Presented) The computer system of claim 59, wherein the tests to determine the interaction between compounds in the first database and the targets in the second database measure functional activity.

77. (Previously Presented) The computer system of claim 59, wherein the tests used to generate results comprising the third database measure adenylyl cyclase activity, inositol triphosphate, or neurotransmitter transport.

78. (Previously Presented) The computer system of claim 59, wherein the tests used to generate results comprising the third database are based on reporter gene assays or functional assays.

79. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as numerical values.

80. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as per cent inhibition values.

81. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as potency values.

82. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values exceed a specified threshold.

83. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values fall below a specified threshold.

84. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values fall between specified upper and lower thresholds.

85. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of profiles of numerical values or meeting specified threshold criteria for specific compounds from the first database with respect to panels of molecular targets in the second database.

86. (Previously Presented) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of profiles of numerical values or of meeting specified threshold criteria for specific compounds from the first database with respect to panels of molecular targets in the second database and in formats that allow comparisons to be made (a) between such profiles among subsets of compounds in the first database or (b) between such profiles or groups of profiles of compounds in the first database and a comparable profile of interaction data for a compound or group of compounds not in the first database.

87. (Previously Presented) The computer system of claim 59, wherein the chemical compounds in the first database are selected from among the compound set comprising LOPAC (List Of Pharmacologically Active Compounds, Sigma/RBI).

88. (Previously Presented) The computer system of claim 59, wherein the chemical compounds in the first database are selected from among the compound set contained in United States Pharmacopeial Convention Inc.'s USP DI Series.

89. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include at least one of the following:

chemical name;

chemical formula;

chemical structure;  
molecular weight;  
physical chemical properties;  
chemical space coordinates;  
chemical structural descriptors;  
solubility; and  
logP.

90. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that can be searched and analyzed using computer-based searching and data analysis methods.

91. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database are organized by chemical structural relatedness or as chemical descriptor arrays or tables.

92. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that can be analyzed using methods of recursive partitioning.

93. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical



structural descriptors that are organized in a format amenable to data analysis using CoMFA software or related methods.

94. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that are organized in a format amenable to data analysis using Catalyst/Hypo software or related methods.

95. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include SMILES codes.

96. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include 2-D topological descriptors.

97. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include 3-D pharmacophore descriptors.

98. (Previously Presented) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include substructure or chemical moiety descriptors.

99. (Previously Presented) The computer system of claim 59, wherein the first database also contains records corresponding to biological information related to effects of the chemical compounds on biological systems.

100. (Previously Presented) The computer system of claim 99, wherein the records in the first database corresponding to biological information includes information on chemical name, trade names, or alternative compound names and at least one of the following categories:

- toxicity;
- side effects;
- mechanism of action; and
- pharmacokinetics.

101. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to pharmacokinetic effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

- bioavailability;
- absorption;
- drug distribution;
- drug metabolism;
- drug excretion;
- blood-protein binding; and

blood-brain barrier passage.

102. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to toxicological effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

teratotoxicity;  
mutagenicity; and  
toxicity.

103. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to side effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

known receptor interactions;  
known enzyme interactions;  
behavioral effect;  
physiological effect; and  
organ effects.

104. (Previously Presented) The computer system of claim 100, wherein records in the first database corresponding to biological information related to

mechanism of action of selected chemical compounds on biological systems includes information on at least one of the following categories:

- target organ;
- major pathway;
- minor pathway; and
- putative molecular target for mode of action.

105. (Previously Presented) The computer system of claim 99, wherein records corresponding to biological information related to effects of the chemical compounds on biological systems can be searched and analyzed using computer-based searching and data analysis methods.

106. (Canceled)

107. (Previously Presented) The computer system of claim 99, wherein records corresponding to biological information related to effects of the chemical compounds on biological systems are encoded using numerical terms such as LD50, ED50, percent absorbed, half-life, and peak concentration.

108. (Previously Presented) The computer system of claim 59, wherein the targets in the second database are selected from among those comprising the superfamily of G-Protein Coupled Receptors, including the following types and subtypes: dopamine, serotonin, adrenergic, muscarinic/acetylcholine, histamine,

adenosine, angiotensin, bradykinin, C5a, chemokine, CCK, endothelin, neuropeptide Y, neurotensin, opioid, somatostatin, tachykinin, vasopressin, galanin, prostanoid, cannabinoid, platelet-activating factor, thyrotropin releasing factor, leukotriene, corticotropin releasing factor, PACAP, vasoactive intestinal peptide, melatonin, glutamate, and GABA-B.

109. (Canceled)

110. (Previously Presented) The computer system of claim 59, wherein the targets in the second database are selected from among those non-steroidal or steroidal intracellular receptors, including estrogen, glucocorticoid, progesterone, and testosterone.

111. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database comprise kinases or phosphatases.

112. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising cytochrome P450 enzymes.

113. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising DNA-modifying enzymes or transferases.

114. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising neurotransmitter-related enzymes.

115. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database comprise proteases or carbohydrates.

116. (Withdrawn) The computer system of claim 69, wherein the molecular targets related to drug discovery and development include nucleic acids.

117. (Withdrawn) The computer system of claim 69, wherein the molecular targets related to drug discovery and development include carbohydrates.

118. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among sodium, potassium, calcium, chloride, or ligand-gated channels.

119. (Withdrawn) The computer system of claim 59, wherein the molecular targets in the second database are selected from among transporters or uptake sites for dopamine, serotonin, norepinephrine, adenosine, glycine, glutamate, and choline.

120. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database include at least one of the following:

- molecular target name;
- molecular target family, classification or type;
- corresponding gene DNA sequence;
- amino acid sequence;
- 3-dimensional conformation or structure;
- location of expression in tissues or cell types;
- hydropathy plots; and
- biochemical or molecular descriptors.

121. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized in a format amenable to computer-based searching and data analysis methods.

122. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by DNA sequence alignments.

123. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by DNA sequence homology.

124. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are grouped by family, superfamily, or subfamily.

125. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by species source of the molecular target used in the test to determine the interaction between chemicals and targets.

126. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by location of expression in tissues.

127. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by major or minor pathways.

128. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by distribution of molecular target protein expression across different cell types.



129. (Previously Presented) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by distribution of location of expression or across different cell types.

130. (Canceled)

131. (Canceled)

132. (Previously Presented) A computer system comprising:

- a first database containing records corresponding to a plurality of chemical compounds,
- a second database containing records corresponding to a plurality of molecular targets;
- a third database containing records corresponding to the results of tests to determine the interaction between compounds in the first database and targets in the second database, wherein the third database includes records corresponding to the results of tests to determine the interaction between all possible combinations of the compounds selected to comprise a compound set in the first database and the molecular targets selected to comprise a molecular target set in the second database;
- and
- a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first

database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.

133. (Currently Amended) A memory for storing data for access by a process being executed by a processor, the memory comprising:

a data structure for maintaining information identifying a plurality of chemical compounds and a plurality of molecular targets, wherein the data structure further maintains a set of information corresponding to results of tests to determine the interaction between each of a plurality of chemical compounds from the identified chemical compounds and each of a plurality of molecular targets from the identified molecular targets, the tests including information on the effect that a compound selected from the identified compounds has on the interaction between a reference compound known to interact with a selected molecular target from the identified molecular targets and said selected molecular target, and

wherein the process provides selected result information based on a request associated with a selected chemical compound or molecular target.

134. (Previously Presented) The memory of claim 133, wherein the chemical compounds are known biologically active chemical compounds.

135. (Previously Presented) The memory of claim 133, wherein the results are represented in a form that reflects whether each chemical compound binds with a corresponding molecular target.

136. (Previously Presented) The memory of claim 133, wherein the results are represented in a form that reflects a potency of a binding between each chemical compound and a corresponding molecular target.

137. (Currently Amended) The memory of claim 133, wherein the data structure maintains a set of information corresponding to results of tests to determine the interaction between ~~all or substantially~~ all of a plurality of compounds selected to comprise a compound set in a chemical compound data structure and ~~all or substantially~~ all of a plurality of molecular targets selected to comprise a molecular target set in a molecular target data structure.

138. (Previously Presented) The memory of claim 133, wherein the data structure maintains a set of information corresponding to results of tests to determine the interaction between a majority of a plurality of compounds selected to comprise a compound set in a chemical compound data structure and a majority of a plurality of molecular targets selected to comprise a molecular target set in a molecular target data structure.

139. (Currently Amended) A computer system comprising:  
a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to screening results from tests of interactions between each of a plurality of compounds in the first database and each of a plurality of molecular targets in the second database, the tests including information on the effect that a compound selected from the first database has on the interaction between a reference compound known to interact with a selected molecular target from the second database and said selected molecular target; and

a user interface allowing a user to view the selected compound and to selectively view information from the first database, the second database, and the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database,

wherein a process ~~identifies~~ provides information reflecting a new relationship between one or more compounds in the first database and one or more targets in the second database, the provided information being relevant to a predictability of a potential use of a new compound.

140. (Currently Amended) The computer system of claim 139, wherein the new relationship is ~~identified~~ provided to determine correlations that are useful for drug discovery and development.

141. (Currently Amended) The computer system of claim 139, wherein the ~~new~~ relationship is ~~identified~~ provided to determine patterns that are useful for drug discovery and development.

142. (Previously Presented) A computer system comprising:

- a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems, wherein the first database includes a database of chemical compounds that have failed in preclinical or human clinical tests;
- a second database containing records corresponding to a plurality of molecular targets;
- a third database containing records corresponding to tests of interactions between compounds in the first database and molecular targets in the second database, the tests including information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target; and
- a user interface allowing a user to view the selected compound and to selectively view information from the first database, the second database, and the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database.

143. (New) A memory for storing data for access by a process being executed by a processor, the memory comprising:

a data structure for maintaining (i) a first set of information associated with one or more chemical compounds, (ii) a second set of information associated with one or more molecular targets, and (iii) a third set of information reflecting interactions between each of a plurality of the chemical compounds and each of a plurality of the molecular targets, wherein the process may provide, based on one or more queries, information reflecting a relationship between a chemical compound included in the first set, a molecular target included in the second set, and the information included in the third set, and wherein the information reflecting the relationship is used to validate disease relevance or biological function of a new molecular target.

144. (New) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds, wherein the chemical compounds in the first database are selected from among the compound set contained in United States Pharmacopeial Convention Inc.'s USP DI Series;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to the results of tests to determine the interaction between each of a plurality of compounds in the first database and each of a plurality of targets in the second database; and

a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first

database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.

145. (New) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds, wherein records corresponding to the chemical compounds in the first database include SMILES codes;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to the results of tests to determine the interaction between each of a plurality of compounds in the first database and each of a plurality of targets in the second database; and

a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.